HW6 solution

MTLE-6120: Spring 2023

Due: Mar 3, 2023

1. **Resistivity of the best conductors**

   Silver, copper, gold and aluminum are the four best conductors at room temperature among the elemental metals, with resistivities of 16, 17, 23 and 27 nΩm respectively. They are all face-centered cubic metals with lattice constants of 4.09, 3.61, 4.08 and 4.05 Å respectively.

   (a) Assuming these are free electron metals, calculate the carrier density, Fermi energy, Fermi velocity and density of states at the Fermi level for all four of them. If the relaxation time τ had been equal for all four, which should have been the best conductor?

   Based on the valence configurations $d^{10}s^1$ for the noble metals and s^2p^1 for Al, these will be free electron metals with $Z_{\text{val}} = 1$ and 3 valence electrons per unit cell respectively. The carrier density is then $n = 4Z_{\text{val}}/a^3$, because of 4 atoms per cubic unit in FCC. From this we canculate $k_F = (3\pi^2 n)^{1/3}$, $v_F = \hbar k_F/m$ and $E_F = mv_F^2/2$, with $m =$ the free electron mass for a free electron model. The density of states at the Fermi level is $mk_F/(\hbar^2\pi^2)$. Evaluating the above expressions, we find

Metal	n [nm^{-3}]	v_F [10^6 m/s]	E_F [eV]	$g(E_F)$ [eV^{-1}nm^{-3}]
Ag	58	1.4	5.5	15.9
Cu	85	1.6	7.1	18.0
Au	59	1.4	5.5	15.9
Al	181	2.0	11.7	23.2

   The conductivity is proportional to $g(E_F)v_F^2$, and both $g(E_F)$ and $v_F \propto k_F$ for a free electron model, so that $\sigma \propto k_F^3 \propto n$. In fact, for a free electron model, Drude theory continues to hold, so that $\sigma = ne^2\tau/m$. Aluminum has the highest n, followed by copper, so if tau had remained the same, those two should have been the best conductors.

   (b) Calculate the τ based on the experimental resistivity numbers given above. What other material properties could one look at to explain this trend?

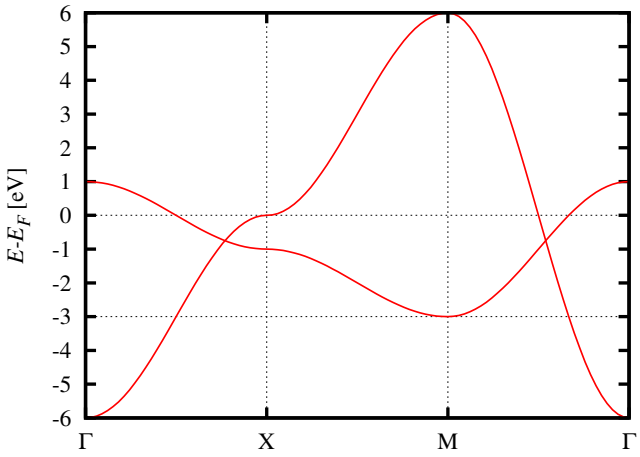
   Using the Drude formula, which remains exactly valid for a quantum free electron model, we can calculate $\tau = m/(\rho ne^2)$ with the results:

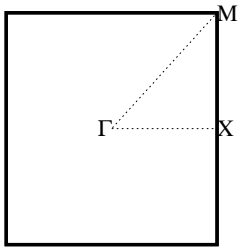
Metal	ρ [nΩm]	n [nm^{-3}]	τ [fs]
Ag	16	58	37
Cu	17	85	24
Au	23	59	26
Al	27	181	7

   This variation of τ depends on many factors. As discussed in class, Fermi golden rule for e-ph scattering rate $\propto g(E_F)$ so the high DOS in Al and then Cu decrease the relaxation time τ. The remaining variation in τ results from the phonon properties. Al has low elastic moduli, which results in larger amplitude phonons for the same energy and stronger e-ph coupling ($c_{\text{e-ph}}$ in our derivation). Au is heavy, which results in a low sound velocity and hence low energy phonons (low Debye temperature), which can be more easily excited at the same temperature, enhancing the Bose occupation factors in the scattering rate and reducing τ. Essentially, a light and high-modulus material will have the largest τ.

2. **Fermi surface and density of states from band structure**

Consider the following band structure of a 2D metal with a simple square lattice. The Brillouin zone and k-path are shown in the right panel.





(a) How many bands are present in this band structure? Identify their energy ranges.

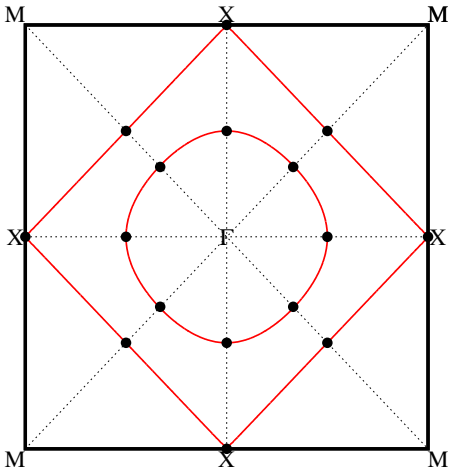
There are two bands: a wide band extending from -6 to $+6$ eV (width 12 eV), and a narrower band extending from -3 to $+1$ eV (width 4 eV).

(b) Plot the Fermi surface of this metal on the Brillouin zone. (Hint: find the points where $E = E_F$ on the band structure, mark them on the Brillouin zone, use symmetries and play connect the dots!)

There are 4 points where $E = E_F$:

- Midpoint of Γ-X
- X
- Midpoint of Γ-M
- 1/3 of the way from Γ-M

Mark these points on the Brillouin zone, but use 4-fold symmetries of square lattice, so that there are 4 copies each of X and M. Connect them up judiciously to get the Fermi surface. Note that both bands cross zero energy, which gives two branches to the Fermi surface.



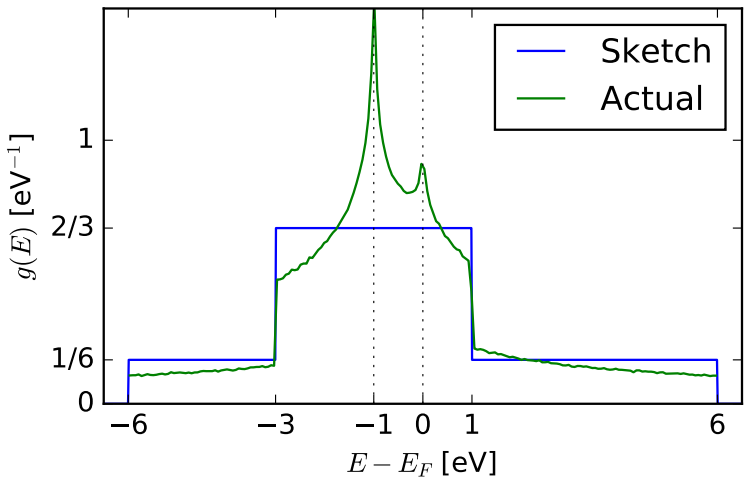
(c) What is total number of states per unit cell?

Each band should have two states per unit cell (accounting for spin). So the total number of states per unit cell is 4.

(d) Sketch the density of states per unit cell as a function of energy. Try to make both axes of the plot as quantitative as possible.

Each band integrates to 2 states per unit cell. These states are within a three times smaller energy range for the narrow band, so its DOS contribution should be typically three times higher than the wide band.

Furthermore, this is 2D, so the density of states for a parabolic band is constant with energy. So essentially the wide band gives 2/12 eV^{-1} from -6 to $+6$ eV, and the narrow band gives 2/4 eV^{-1} from -3 to $+1$ eV. Adding these two, we have 1/6 eV^{-1} from -6 to $+6$ eV, except for $1/6 + 1/2 = 2/3$ eV^{-1} from -3 to $+1$ eV, which gives the plot:



For reference, I have also shown the actual density of states from the model I used to construct the band structure for comparison. Note the spikes at 0 and -1 eV: these correspond to the flat sections in the center of each band at the X point of the band structure. We could have also guessed this part, but we got quite close with just the simple considerations above.

3. **Fermi theory properties of a metal in 2D**

Consider a simple metal in 2D containing n_{ion} ions per unit area. For all questions asking for a 'dependence' below, only predict the power law eg. explain why something is T^3 (say), without worrying about the prefactor.

(a) What is the temperature dependence of electronic heat capacity for $T \ll T_F$?

The Fermi theory arguments for $T \ll T_F$ work regardless of the electronic DOS details. Nothing changes in going from 2D to 3D, and $C_V \propto T$ for electrons.

(b) What is the frequency dependence of the phonon density of states $g(\omega)$ in the Debye model?

As derived in class, the density of states of phonons with linear dispersion is $\propto \omega^{d-1}$ i.e. $\propto \omega$. This is cutoff at the Debye frequency ω_D, so the overall frequency dependence is $g(\omega) \propto \omega\Theta(\omega_D - \omega)$.

(c) What is the temperature dependence of the lattice heat capacity for $T \ll T_D$?

Compared to the derivation for the 3D case in class, all that changes is you have one less power of ω in the phonon density of states and hence the internal energy integral. In the $T \ll T_D$ limit, this gives one fewer power of T, which yields $C_V \propto T^2$.

(d) What is the lattice heat capacity per unit area for $T \gg T_D$? (Give absolute expression.)

Equipartition theorem applies, so $C_V = 2n_{\text{ion}}k_B$. Note 2 instead of 3, because you have 2 degrees of freedom per ion now, instead of 3.

(e) What is the temperature dependence of electronic resistivity for $T \ll T_D$?

The phonon density of states has one fewer power of ω, so the Fermi Golden rule integral has one fewer power too. In the $T \ll T_D$ limit, this gives one fewer power of T than the 3D case, i.e. $\rho \propto T^4$

(f) What is the temperature dependence of electronic resistivity for $T \gg T_D$?

For $T \gg T_D$, equipartition applies to phonons, so phonon DOS is irrelevant. Therefore the temperature dependence is same as 3D i.e. $\rho \propto T$.